Method of Constrained Global Optimization

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We present a new method for optimization: constrained global optimization (CGO). CGO iteratively uses a Glauber spin flip probability and the Metropolis algorithm. The spin flip probability allows changing only the values of variables contributing excessively to the function to be minimized. We illustrate CGO with two problems—Thomson's problem of finding the minimum–energy configuration of unit charges on a spherical surface, and a problem of assigning offices—for which CGO finds better minima than other methods. We think CGO will apply to a wide class of optimization problems.

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Introduction   Optimization problems are important in the physical sciences [1,2], biological sciences [3], mathematics [4], and operations research [5]. Current methods for approaching optimization problems include Monte Carlo simulation, analytic methods, symmetry considerations, and the method of simulated annealing (SA) [5]. Here we present a new method for optimization— the method of constrained global optimization (CGO). CGO, like SA, makes iterative use of the Metropolis algorithm [6]. CGO uses a Glauber spin flip probability to insure in general that only those variables making excessively large contributions to the function to be minimized are assigned new values at a given iteration, while the values of the other variables remain the same. SA changes the values of one or more randomly–selected variables at each iteration.

We first describe CGO, then illustrate its use on two problems— Thomson's Problem of finding the configuration of unit charges on a the surface of a sphere with minimum potential energy, and the office assignment problem (OAP)—for which CGO obtained better results than other methods.

Description of Method of Constrained Global Optimization   Let f be a real valued function of the N variables $x_1, x_2, x_3, \ldots, x_N$. We seek to find the values of $x_1, \ldots, x_N$ which will minimize $f(x_1, \ldots, x_N)$. We denote $(x_1, x_2, x_3, \ldots, x_N)$ by $\mathbf{x}$. The set of allowed values of $\mathbf{x}$ may be infinite (discrete or continuous) or finite.

First begin with some randomly (or otherwise) chosen initial values for the variables, denoted by $\mathbf{x}^0$. After this, CGO consists of a three–step process which is iterated some given number of times.

Step (1): Determine, for each variable x_i, whether $x_i^{(n+1)}$ is to remain equal to x_i^n or to change to some other value. Select a random number R_i between 0 and 1. If

$$R_i < 1/(1 + exp(-(g(x_i^n) - C)/kT)) \tag{1}$$

then as described in step (2) a new value will be selected for x_i; otherwise, $x_i^{(n+1)}$ will remain equal to x_i^n. In Eq. (1) g is a real–valued function of x_i; C is a real number used for all x_i^n for one iteration but which may change each iteration; k is a constant (Boltzmann constant); T is the "temperature" of the system. The right side of Eq. (1) is the Glauber probability of a spin flip and is derived by considering each $x_i^{(n+1)}$ to have two states: remaining equal to x_i^n or not. Then by solving $P_= + P_{\neq} = 1$, and $P_=/P_{\neq} = exp(-g(x_i^n)/kT)/exp(-C/kT)$ for $P_{\neq}$ we get equation (1).

We can consider $g(x_i^n)$ to be an "energy" associated with $x_i^{(n+1)}$ remaining equal to x_i^n, and C a threshold energy associated with selecting a new value for $x_i^{(n+1)}$. The choice of the function g and the constant C are problem–dependent. For problems based on particle interactions obeying a linear superposition principle a clear choice is to take g so that $f = \sum_{i=1}^{N} g(x_i)$. For problems in which f is not derived from a superposition principle one should attempt to choose g so as to divide the "cost" of f among the variables. The value of C at a given iteration may depend on the current values of the variables. In general, increasing C decreases the probability that variables will change values; decreasing C increases the probability.

Step (2): For each x_i^n determined to remain unchanged in step (1), set $x_i^{(n+1)} = x_i^n$. For each x_i^n determined to change in step (1), choose a new $x_i^{(n+1)}$ randomly from the set of allowed values. The set of allowed values is problem dependent. For example, certain problems may limit the number of variables x_i which can have the same value. If this is true then special care must be taken in choosing the $\{x_i^{(n+1)}\}$. One such procedure for doing this is illustrated for the office assignment problem below.

Step (3):   Calculate $f(\mathbf{x}^{(n+1)})$ and perform the Metropolis algorithm: If $f(\mathbf{x}^{(n+1)}) < f(\mathbf{x}^n)$ then the new arrangement is accepted. If $f(\mathbf{x}^{(n+1)}) \geq f(\mathbf{x}^n)$ then

the new arrangement is rejected unless a random number R which is selected is less than $\exp(-(f(\mathbf{x}^{(n+1)}) - f(\mathbf{x}^n))/T)$; if the new arrangement is rejected, $x_i^{(n+1)}$ is set back to x_i^n for all i.

The three–step process is iterated a certain number of times at a given temperature, and then the temperature is lowered according to some annealing schedule and the process iterated at that temperature. Eventually the temperature becomes so low that the values of the variables $\{x_i\}$ become frozen in.

Step (2) allows for potentially global rearrangements of a system, but these arrangements are constrained by step (1) which in general only allows those variables with excessively large energies to change values. Also, rearrangements are ultimately limited by step (3), which in general does not allow moves to values of $\mathbf{x}$ with larger values of f. CGO differs from SA in steps (1) and (2), and shares the use of the Metropolis algorithm (step (3)) with SA.

Thomson Problem   Consider N point charges on (the surface of) a unit conducting sphere, interacting only through their mutual Coulomb forces. What is the configuration of the charges for which the Coulombic energy $\frac{1}{2}\sum_{i,j=1;j\neq i}^N 1/|\mathbf{r}_i - \mathbf{r}_j|$ is minimized? This question was originally asked by Thomson for $2 \leq N \leq 100$, [4] and has since been investigated by many authors [2,7–10]. Somewhat surprisingly, it turns out that the configuration of minimum energy is not the configuration which places the charges at furthest distance from each other, or the configuration of greatest symmetry. For example, for 8 charges, the configuration of minimum energy is not a cube, but a twisted noncubic rectangular parallelpiped [2].

For Thomson's problem, we take the function g in Eq. (1) equal to $g(\mathbf{r}_i) = \frac{1}{2}\sum_{j=1;j\neq i}^N 1/|\mathbf{r}_i - \mathbf{r}_j|$. For those charges which change coordinates, we assign new spherical coordinates as $\theta_i^{(n+1)} = \theta_i^n + \eta R_i \pi$, $\phi_i^{(n+1)} = \phi_i^n + \eta R_i' 2\pi$ ($r_i \equiv 1, \forall i$); here R_i, and R_i' are random numbers between 0 and 1, η reduces the maximum angular change in proportion to the cooling schedule, and the additions are done with the appropriate periodicity. We use $C = \lambda \cdot \max\{g(\mathbf{r}_i)|i = 1, 2, \ldots, N\}$ with $\lambda = 0.7$; the results are not very sensitive to small changes from this value of λ. At each temperature step we consider 100 configurations (iterations); then we lower the temperature T used in Eq. (1), the Metropolis algorithm, and η, by a factor of 0.9. Finally, we use the final configuration from CGO as input to a conjugate gradient descent algorithm to reduce the energy as far as possible, using double–precision arithmetic. We repeated the entire procedure from five different starting configurations for each number of charges.

Our results using CGO for $2 \leq N \leq 65$ confirm the minimum energy values found previously [7]. We find improvements in previously–found minimum energy values

for most values of N between 66 and 100. We list values we believe to be the minimum energies for $66 \leq N \leq 100$ in table I.

For some numbers of charges the minimum energy obtained by CGO is lower than that obtained by using SA [8], by Monte Carlo simulation [9], or by finding the configuration of minimum energy with a given symmetry [10]. In particular, these results demonstrate that the symmetry of the configuration of minimum energy is not always obvious *a priori*. The output from CGO is typically well within one tenth of one percent of the final minimum energy after applying the conjugate gradient, and this performance of CGO relative to final minimum energy value does not deteriorate with increasing N. We think that CGO will be readily applicable to other ionic and molecular structure problems.

Office Assignment Problem   Consider a set of N offices whose centers are located at the 2D coordinates $\{\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\}$. These are to be occupied by N people whose interactions—coefficients of angst—are denoted by $\{a_{ij}|i, j = 1, 2, \ldots, N\}$. We seek to minimize the function

$$A = \sum_{i,j=1;i\neq j}^N a_{ij}/|\mathbf{r}(i) - \mathbf{r}(j)|\,,$$

which one can interpret as the total angst of the system. Here, $\mathbf{r}(i)$ is the location of the ith person's office, which must be one member of the set $\{\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\}$

For step (1) of CGO, we take

$$g(\mathbf{r}(i)) \equiv A_i = \sum_{j=1;j\neq i}^N a_{ij}/|\mathbf{r}(i) - \mathbf{r}(j)|,$$

which can be considered as the angst felt by individual person i. We take $C = \lambda \cdot \max\{A_i|i = 1, 2, \ldots, N\}$ with $\lambda = 1.2$ (With a_{ij} values as defined below, the results degrade significantly for λ above 2.0.) For this problem with g thus defined, step (1) of CGO insures that only people who are relatively "unhappy" with their office want to find a new office, while those who are happy with their office don't want to move. For step (2) of CGO, we permute those people who want new offices in a random fashion: Choose a random number for each person who wants a new office. Sort these random numbers, and shadow the sort operations on their office assignments.

We consider problems with 20, 30, 40, 60, and 100 people. We use random locations $\mathbf{r}_i$ in the unit square, and we choose the a_{ij} randomly between -1 and +1 with $a_{ij} = a_{ji}$ and $a_{ii} = 0$. We attempt to find the minimum value of A using CGO and SA with the rearrangement suggested by Lin and Kernighan [11]. For a given number of people we start both methods from ten different starting configurations. Both methods use the same annealing schedule [12]. We try up to $100N$ arrangements at a given temperature, stopping if $10N$ successful moves

occur at a given temperature. Then we lower the temperature by a factor of T_1. At the Mth annealing step, the temperature is $T = T_0(T_1)^M$, where T_0 is the initial temperature. For the runs reported here, we use T_0 and $T_1 = 0.9$; we anneal for 40 annealing steps, at which temperature the configurations for both methods were frozen in.

We give results in table II. CGO finds significantly lower values of A, both minimum and mean, than SA using the Lin–Kernighan rearrangement. The CGO runs take about two–thirds the computer time of the SA runs. We have annealed up to 100 times more slowly for some cases without altering the qualitative results of table II.

The Lin–Kernighan rearrangement works exceptionally well for the traveling salesperson problem (TSP), but appears to have difficulties for the OAP. For the TSP the only relevant distances are those between a city and its neighbors, while in the OAP a person must consider all of the other people, not just neighbors. Perhaps, the Lin–Kernighan rearrangement is optimal for the TSP because it allows consideration of changes in distances to neighbors at the endpoints of a segment while leaving distances for other cities unaffected. But for the OAP changes in angst for people at the endpoints of the reversed or transported segment cannot be considered independently of the changes in angst for other people. CGO provides an effective method for moving unhappy people, while leaving the happy ones where they are.

Conclusion We have used CGO to improve known values of the minimum potential for Thomson's problem for many numbers of charges from 66 to 100. For the office assignment problem CGO found significantly lower results than SA. We think that CGO will be applicable to a wide class of optimization problems, especially those with long range interactions.

[1] R. Rafac, J. P. Schiffer, J. S. Hangst, D. H. E. Dubin, and D. J. Wales, Proc. Natl. Acad. Sci USA **88** 483 (1991).
[2] L. T. Wille, Nature **324** 46 (1986).
[3] G. S. Mageras and R. Mohan, Med. Phys. **20** 639 (1993).
[4] L. L. Whyte, AM. Math. Mnthly. **59** 606 (1952).
[5] S. Kirkpatrick, C. D. Gelatt, Jr., and M. P. Vecchi, Science **220** 671 (1983).
[6] N.Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, and E. Teller, J. Chem. Phys **21** 1087 (1953).
[7] T. Erber and G. M. Hockney, J. Phys. A **24**, L1369 (1991).
[8] J. R. Edmunsen, Acta Cryst. A**48**, 60 (1992).
[9] L. Glasser and A. G. Avery, J. Phys. A **25**, 2473 (1992).
[10] J. R. Edmunsen, Acta Cryst. A**49**, 648 (1993).
[11] S. Lin, Bell Syst. Tech. J. **44** 2245 (1965); S. Lin and B. W. Kernighan, Oper. Res. **21** 498 (1973).
[12] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge, New York, 1990).

TABLE I. Values obtained using the method of constrained global optimization that we believe to be minimum Coulombic energies for Thomson's problem of N unit point charges on the surface of a unit sphere.

N	Energy[a]	N	Energy
66	1882.441525[b]	84	3103.465124[b,c]
67	1942.122700	85	3180.361443[c]
68	2002.874702[b]	86	3258.213663[b]
69	2064.536066[c]	87	3337.002643
70	2127.100902[b,c]	88	3416.720197[b]
71	2190.649906[c]	89	3497.439019
72	2255.001191	90	3579.091223[b,c]
73	2320.633884	91	3661.713699
74	2387.072982[b]	92	3745.291636[b,e]
75	2454.369689	93	3829.844338
76	2522.674872[b]	94	3915.309270[b]
77	2591.850152	95	4001.771676
78	2662.046475[d]	96	4089.154010[b]
79	2733.248358[c]	97	4177.533600
80	2805.355876[b,c]	98	4266.822464[b]
81	2878.522830[c]	99	4357.139163[c]
82	2952.569675[b,c]	100	4448.350634
83	3027.528489[c]		

[a]Coordinates available; contact ELA.
[b]Improves minimum energy value found in ref. [10], which used symmetry considerations.
[c]Improves minimum energy value found in ref. [9], which used a Monte Carlo method.
[d]From Ref. [10]; CGO found 2662.047213.
[e]Improves minimum energy value found in ref. [8], which used simulated annealing.

TABLE II. Comparison of angst values for the office assignment problem using the method of constrained global optimization (CGO) and simulated annealing with the Lin–Kernighan rearrangement (SA). N is the number of offices, which is equal to the number of occupants. The column labelled "minimum" is the lowest value from ten runs using different initial conditions; the column labelled "mean" is the average of the ten values.

N	CGO		SA	
---	minimum	mean	minimum	mean
20	-9.4698	-9.2212	-9.1134	-8.5286
30	-45.4959	-40.1290	-41.9456	-36.8261
40	-29.3538	-26.8098	-20.2484	-19.3516
60	-77.9358	-73.6713	-63.2809	-60.3534
100	-144.8887	-139.8323	-108.6005	-100.4544